

Electronic Supporting Information

Correlating Experimental Electrochemistry and Theoretical Calculations in 2'-Hydroxy Chalcones Derivatives: The Role of Intramolecular Hydrogen Bond

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Figure s1. SOMO (singly occupied molecular orbital) for the anion radicals of chalcones 1-6.

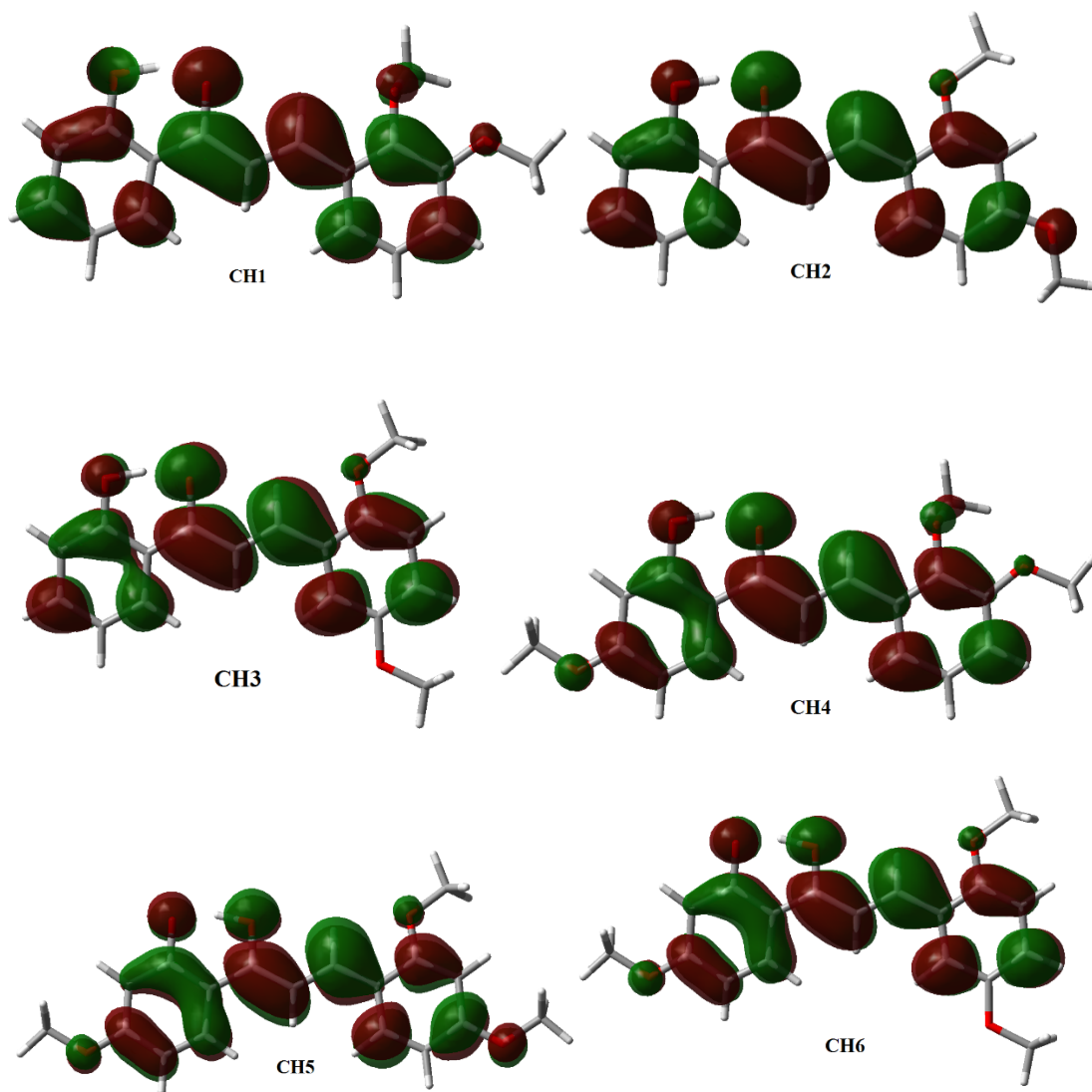
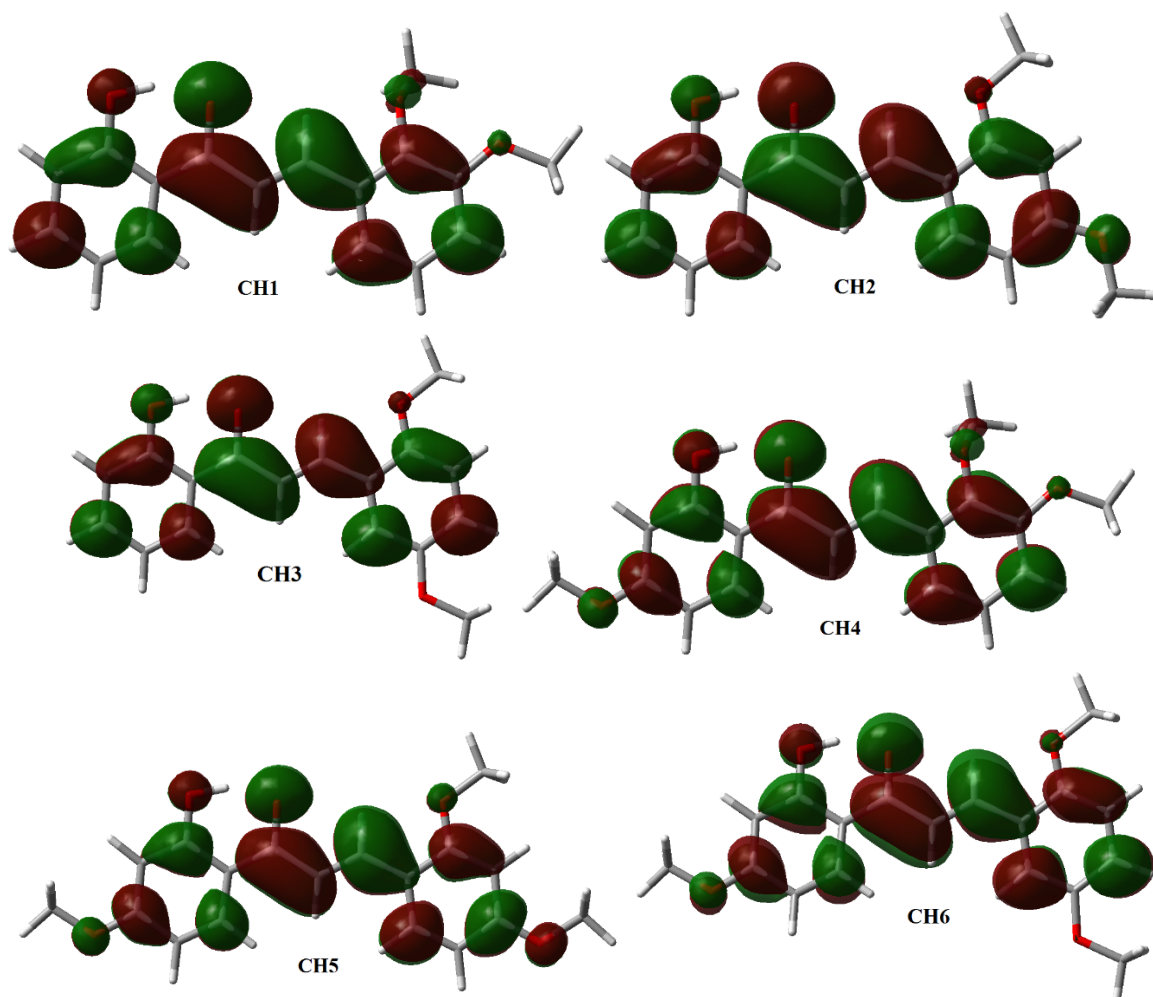


Figure s2. SOMO for the vertical attachment electron of anion radicals of chalcones 1-6.



Optimized geometries and energies.

DFT B3P86/6-31+G(d,p) level, C-PCM(DMSO)

Neutral species

Ch1 (neutral)

C	-5.846614	-0.238385	0.009902
C	-6.017401	1.128238	0.162995
C	-4.909088	1.985387	0.228024
C	-3.632945	1.457253	0.137911
C	-3.417473	0.071397	-0.018404
C	-4.557080	-0.779366	-0.081720
H	-6.698108	-0.914318	-0.041658
H	-7.024763	1.536695	0.233209
H	-5.048526	3.057388	0.348066
H	-2.786881	2.137312	0.191008
C	-2.078801	-0.525723	-0.116029
C	-0.882223	0.315037	-0.057385
C	0.346974	-0.242135	-0.130366
C	1.622038	0.454664	-0.083814
C	2.803364	-0.309360	-0.129098
C	1.725953	1.858492	0.001827
C	4.066695	0.318160	-0.096519
C	2.967315	2.466532	0.049672
H	0.827144	2.470053	0.030630
C	4.142132	1.706265	0.001986
H	3.040913	3.550199	0.119033
H	5.102450	2.211876	0.030324
H	-1.002413	1.388635	0.049192
H	0.399996	-1.322601	-0.235250
O	-1.966366	-1.771006	-0.251198
O	-4.437960	-2.105483	-0.228041
H	-3.447966	-2.284307	-0.271378
O	2.725499	-1.666600	-0.271155
O	5.136934	-0.510345	-0.179214
C	3.089590	-2.422777	0.890753
H	4.121646	-2.214058	1.183866

H	2.408737	-2.195345	1.718930
H	2.989165	-3.472759	0.612913
C	6.433553	0.070172	-0.131274
H	6.591678	0.754136	-0.972768
H	6.592645	0.603626	0.812696
H	7.133513	-0.762164	-0.202723

Neutral

E = -961.074457971 Hartree

Zero-point correction = 0.293110 (Hartree/Particle)

Radical anion optimized at neutral geometry

E = -961.203719525 Hartree

Zero-point correction = 0.290620 (Hartree/Particle)

Ch2 (neutral)

C	-5.874329	-0.244229	0.005644
C	-5.859336	-1.630012	0.014770
C	-4.645059	-2.331507	0.016194
C	-3.451873	-1.629026	0.008235
C	-3.425329	-0.218718	-0.001460
C	-4.669677	0.472137	-0.002487
H	-6.809573	0.312915	0.004497
H	-6.802332	-2.175499	0.020969
H	-4.637695	-3.419318	0.023401
H	-2.521039	-2.190376	0.009351
C	-2.177311	0.562119	-0.010169
C	-0.883717	-0.104640	-0.007833
C	0.261472	0.624427	-0.008033
C	1.617487	0.130300	-0.005424
C	2.702452	1.054305	0.003288
C	1.938427	-1.236687	-0.011340
C	4.018447	0.608097	0.006101
C	3.244879	-1.701165	-0.008893
H	1.134269	-1.970211	-0.018805
C	4.289395	-0.766239	0.000079
H	3.431939	-2.769559	-0.014114

H	-0.854934	-1.189771	-0.004271
H	0.150054	1.705562	-0.009548
O	-2.245291	1.822082	-0.018932
O	-4.729540	1.810970	-0.011293
H	-3.767197	2.117477	-0.015952
O	2.368387	2.363816	0.009002
C	3.406559	3.335563	0.019232
H	4.026303	3.239731	0.917473
H	4.033749	3.250903	-0.874968
H	2.904617	4.302853	0.023116
O	5.600549	-1.093522	0.003418
H	4.861445	1.290886	0.012880
C	5.956616	-2.472301	-0.003771
H	7.046028	-2.495654	0.000685
H	5.574710	-2.981307	0.887593
H	5.582203	-2.969947	-0.904667

Neutral

E = -961.085537115 Hartree

Zero-point correction = 0.293376 (Hartree/Particle)

Radical anion optimized at neutral geometry

E = -961.211064259 Hartree

Zero-point correction = 0.290798 (Hartree/Particle)

Ch3 (neutral)

C	-5.689339	-0.290590	0.020579
C	-5.620588	-1.674293	-0.006128
C	-4.380339	-2.328780	-0.034516
C	-3.215154	-1.581707	-0.034680
C	-3.243235	-0.171057	-0.007935
C	-4.513338	0.471635	0.018748
H	-6.645284	0.229752	0.042311
H	-6.541856	-2.255784	-0.005357
H	-4.331809	-3.415312	-0.056272
H	-2.263940	-2.107233	-0.057957
C	-2.028399	0.655931	-0.006288
C	-0.705042	0.035100	-0.010058

C	0.408530	0.803663	-0.005805
C	1.786876	0.348132	-0.003435
C	2.831884	1.310220	-0.006031
C	2.129964	-1.010017	0.002931
C	4.160275	0.889035	-0.002233
C	3.458169	-1.426723	0.006831
H	1.354879	-1.774101	0.005976
C	4.477511	-0.470511	0.004207
H	-0.636462	-1.048401	-0.013055
H	0.264606	1.880546	-0.003361
O	-2.137092	1.910103	0.002126
O	-4.625934	1.806218	0.043766
H	-3.680602	2.154946	0.031213
O	2.454967	2.614294	-0.012595
C	3.468598	3.609260	-0.015329
H	4.093889	3.539557	0.882034
H	4.097146	3.531179	-0.909717
H	2.945152	4.565310	-0.020751
H	4.975548	1.605300	-0.004099
O	3.663118	-2.775640	0.013617
H	5.525466	-0.754823	0.007242
C	5.003585	-3.242845	0.021645
H	4.941028	-4.331157	0.027564
H	5.544685	-2.914278	-0.873522
H	5.537336	-2.904014	0.917408

Neutral

E = -961.080189305 Hartree

Zero-point correction = 0.293235 (Hartree/Particle)

Radical anion optimized at neutral geometry

E = -961.210086872 Hartree

Zero-point correction = 0.290828 (Hartree/Particle)

 CH4 (neutral)

C	5.058847	0.617830	-0.040441
C	5.301771	-0.748982	0.051556

C	4.231826	-1.667971	0.096817
C	2.937971	-1.203628	0.051074
C	2.639113	0.176124	-0.041817
C	3.738699	1.080331	-0.088669
H	5.854059	1.355225	-0.078231
H	4.449635	-2.731142	0.167580
H	2.134398	-1.934761	0.087638
C	1.282362	0.708369	-0.092127
C	0.126546	-0.189432	-0.034245
C	-1.128057	0.307409	-0.100982
C	-2.368891	-0.450350	-0.054271
C	-3.585652	0.252741	-0.130684
C	-2.405444	-1.855249	0.062749
C	-4.816991	-0.435553	-0.100183
C	-3.616070	-2.522786	0.110964
H	-1.477960	-2.420582	0.119370
C	-4.826142	-1.823083	0.031093
H	0.300103	-1.256794	0.063428
H	-1.232663	1.384217	-0.203785
O	1.104300	1.954328	-0.186097
O	3.546226	2.399875	-0.179915
H	2.540807	2.519543	-0.205064
O	-3.572765	1.609353	-0.301592
C	-3.993224	2.369816	0.838167
H	-5.021703	2.122937	1.113315
H	-3.321501	2.186378	1.684510
H	-3.931065	3.418033	0.542837
O	6.534268	-1.294255	0.103155
C	7.665097	-0.429211	0.066673
H	8.537240	-1.079923	0.122427
H	7.690714	0.142134	-0.867342
H	7.661029	0.255864	0.921125
H	-3.637039	-3.606862	0.206687
H	-5.760992	-2.374463	0.060438
O	-5.925227	0.337019	-0.219231
C	-7.192477	-0.301873	-0.141301
H	-7.320542	-0.808167	0.822200
H	-7.931581	0.493345	-0.237399

H -7.323067 -1.022553 -0.956542

Neutral

E = -1075.89511811 Hartree

Zero-point correction = 0.325836 (Hartree/Particle)

Radical anion optimized at neutral geometry

E = -1076.02152935 Hartree

Zero-point correction = 0.324317 (Hartree/Particle)

Ch5 (neutral)

C	5.149155	0.461199	-0.004600
C	5.296402	-0.921786	0.014845
C	4.164853	-1.763764	0.023848
C	2.906222	-1.206796	0.012860
C	2.704107	0.192444	-0.007303
C	3.864152	1.017425	-0.015274
H	5.993790	1.142516	-0.011709
H	4.306326	-2.842045	0.039343
H	2.053170	-1.880403	0.020611
C	1.384591	0.822103	-0.018878
C	0.174932	0.011416	-0.013822
C	-1.048452	0.598617	-0.011332
C	-2.333782	-0.058925	-0.008732
C	-3.521467	0.717463	0.009073
C	-2.481660	-1.460763	-0.025045
C	-4.782126	0.113210	0.009694
C	-3.717103	-2.074285	-0.024525
H	-1.592288	-2.087974	-0.039943
C	-4.875513	-1.280703	-0.007318
H	0.273905	-1.069766	-0.010855
H	-1.068150	1.685247	-0.010815
O	1.304218	2.085391	-0.033292
O	3.764451	2.350785	-0.032995
H	2.765953	2.536794	-0.036704
O	-3.360420	2.059264	0.025945
C	-4.511548	2.894163	0.044735
H	-5.124274	2.741516	-0.850540

H	-5.112127	2.717650	0.943853
H	-4.132905	3.915987	0.055800
H	-5.675852	0.720745	0.023310
O	6.489691	-1.553192	0.026619
C	7.675928	-0.765696	0.017553
H	8.502669	-1.475407	0.029131
H	7.731086	-0.150929	-0.887255
H	7.727905	-0.125356	0.904653
H	-3.813495	-3.157673	-0.037974
O	-6.048645	-1.951218	-0.008776
C	-7.262644	-1.208712	0.006988
H	-7.346980	-0.573981	-0.881999
H	-8.062282	-1.948944	0.002404
H	-7.337093	-0.595887	0.912073

Neutral

E = -1075.90563962 Hartree

Zero-point correction = 0.326160 (Hartree/Particle)

Radical anion optimized at neutral geometry

E = -1076.02826638 Hartree

Zero-point correction = 0.324403 (Hartree/Particle)

Ch6 (neutral)

C	4.950705	-0.410956	-0.056834
C	5.016778	0.969116	0.106553
C	3.837809	1.739072	0.199699
C	2.614049	1.115022	0.128695
C	2.494313	-0.284831	-0.035995
C	3.700528	-1.036718	-0.126684
H	5.833538	-1.037184	-0.132725
H	3.917813	2.816057	0.326768
H	1.723193	1.733066	0.204133
C	1.216443	-0.983943	-0.115837
C	-0.043499	-0.243829	-0.038923
C	-1.225526	-0.898694	-0.082232
C	-2.551489	-0.307123	-0.031429

C	-3.684128	-1.155631	0.085679
C	-2.758191	1.075646	-0.104863
C	-4.962049	-0.601728	0.127416
C	-4.037051	1.625408	-0.061652
H	-1.912132	1.752181	-0.210720
C	-5.143816	0.780782	0.054875
H	-0.009262	0.837354	0.058931
H	-1.188655	-1.981937	-0.157688
O	1.200915	-2.239358	-0.251822
O	3.678250	-2.364042	-0.280294
H	2.695480	-2.609878	-0.299120
O	-3.437163	-2.489221	0.160037
C	-4.543493	-3.374034	0.260615
H	-5.116192	-3.187918	1.176347
H	-5.202652	-3.285003	-0.610529
H	-4.118783	-4.377307	0.294698
H	-5.842007	-1.230044	0.218195
O	-4.108086	2.985415	-0.144758
H	-6.156655	1.170086	0.089092
C	-5.394539	3.584435	-0.119247
H	-5.226665	4.658462	-0.201114
H	-6.007509	3.246647	-0.963300
H	-5.915692	3.368635	0.821042
O	6.169544	1.664737	0.188251
C	7.401457	0.955422	0.103696
H	8.183716	1.708390	0.194909
H	7.491855	0.229690	0.918967
H	7.493130	0.443980	-0.860394

Neutral

E = -1075.90101389 Hartree

Zero-point correction = 0.325902 (Hartree/Particle)

Radical anion optimized at neutral geometry

E = -1076.02780693 Hartree

Zero-point correction = 0.324611 (Hartree/Particle)

Radical anion species

Ch1(radical)

C	-5.859494	-0.202452	-0.024688
C	-6.035204	1.169347	0.132578
C	-4.918474	2.008832	0.221455
C	-3.640151	1.467331	0.151602
C	-3.420385	0.083575	-0.008939
C	-4.573868	-0.753249	-0.095647
H	-6.713704	-0.874550	-0.095323
H	-7.040964	1.583574	0.186498
H	-5.045106	3.082754	0.345710
H	-2.789658	2.141447	0.226158
C	-2.086783	-0.538846	-0.089920
C	-0.900051	0.224411	-0.035647
C	0.370200	-0.331389	-0.102611
C	1.614843	0.390194	-0.067551
C	2.838997	-0.319484	-0.136884
C	1.698793	1.804423	0.029287
C	4.077540	0.342886	-0.116340
C	2.922810	2.449388	0.060266
H	0.786981	2.394658	0.082231
C	4.127014	1.735931	-0.011017
H	2.957742	3.535244	0.138154
H	5.072115	2.268189	0.009283
H	-1.002733	1.300844	0.059823
H	0.438880	-1.410906	-0.193441
O	-2.040520	-1.847256	-0.219919
O	-4.431232	-2.083048	-0.246612
H	-3.365721	-2.191660	-0.257671
O	2.817781	-1.688626	-0.283644
O	5.176593	-0.458764	-0.209314
C	3.104813	-2.407642	0.915982
H	4.110228	-2.172638	1.279436
H	2.364440	-2.173870	1.690494
H	3.045314	-3.468808	0.665983
C	6.451543	0.160688	-0.158524
H	6.591008	0.856498	-0.994229

H	6.597661	0.694449	0.787958
H	7.179694	-0.647346	-0.235569

Radical

E = -961.210490049 Hartree

Zero-point correction = 0.290270 (Hartree/Particle)

Neutral optimized at radical anion geometry

E = -961.064295450 Hartree

Zero-point correction = 0.292213 (Hartree/Particle)

Ch2(radical)

C	5.879911	-0.265481	-0.002395
C	5.869699	-1.657979	-0.005280
C	4.649821	-2.344595	-0.004760
C	3.455860	-1.632301	-0.001670
C	3.424049	-0.222030	0.000776
C	4.680799	0.457755	0.000835
H	6.817060	0.289717	-0.002500
H	6.810541	-2.206439	-0.007758
H	4.630381	-3.432963	-0.006533
H	2.521923	-2.190301	-0.000864
C	2.188102	0.578141	0.003678
C	0.907985	-0.014681	-0.000338
C	-0.273145	0.716864	0.001122
C	-1.609011	0.180888	-0.000099
C	-2.737205	1.059786	-0.002350
C	-1.905637	-1.196490	0.001813
C	-4.037975	0.576438	-0.002476
C	-3.206702	-1.700259	0.001723
H	-1.085487	-1.911313	0.004144
C	-4.277382	-0.807061	-0.000311
H	-3.358218	-2.774873	0.003620
H	0.860404	-1.099416	-0.004991
H	-0.183914	1.798178	0.003842
O	2.322589	1.891147	0.010144
O	4.716337	1.802907	0.003995

H	3.664684	2.050273	0.007479
O	-2.445691	2.390931	-0.004296
C	-3.519763	3.316186	-0.005710
H	-4.143068	3.201572	-0.900513
H	-4.143289	3.204068	0.889258
H	-3.061983	4.305876	-0.007045
O	-5.595172	-1.170001	0.000045
H	-4.897102	1.239131	-0.004079
C	-5.895719	-2.556188	0.004046
H	-6.983691	-2.628467	0.003933
H	-5.497175	-3.052111	-0.889003
H	-5.497686	-3.046748	0.900280

Radical

E = -961.217301360 Hartree

Zero-point correction = 0.290165 (Hartree/Particle)

Neutral optimized at radical anion geometry

E = -961.076649259 Hartree

Zero-point correction = 0.292216 (Hartree/Particle)

Ch3(radical)

C	-5.691942	0.274671	0.001964
C	-5.643924	1.665468	-0.008216
C	-4.406449	2.319964	-0.014783
C	-3.232337	1.575985	-0.011114
C	-3.238791	0.166219	-0.000677
C	-4.511886	-0.479775	0.005664
H	-6.643374	-0.255495	0.007079
H	-6.569804	2.238871	-0.011112
H	-4.358288	3.407326	-0.022846
H	-2.284108	2.108951	-0.016732
C	-2.022219	-0.666820	0.003801
C	-0.727315	-0.105592	-0.000884
C	0.431553	-0.872489	0.000279
C	1.781102	-0.378433	-0.000823
C	2.877838	-1.296637	-0.003204

C	2.104861	0.993893	0.001218
C	4.187103	-0.839892	-0.003302
C	3.423684	1.446737	0.001115
H	1.314039	1.740700	0.003839
C	4.478794	0.535037	-0.001102
H	-0.649254	0.977172	-0.005648
H	0.309952	-1.950436	0.002776
O	-2.189388	-1.971375	0.012230
O	-4.585875	-1.823301	0.015074
H	-3.550791	-2.101410	0.014871
O	2.541120	-2.623312	-0.005248
C	3.590492	-3.573814	-0.011062
H	4.216156	-3.473742	-0.906618
H	4.220325	-3.480385	0.882297
H	3.109879	-4.552888	-0.013484
H	5.019025	-1.536907	-0.005060
O	3.582842	2.809436	0.003349
H	5.516621	0.850748	-0.001175
C	4.905500	3.317327	0.012045
H	4.812033	4.403908	0.016363
H	5.451328	2.996393	0.907685
H	5.460275	3.004511	-0.880983

Radical

E = -961.216248368 Hartree

Zero-point correction = 0.290494 (Hartree/Particle)

Neutral optimized at radical anion geometry

E = -961.070599213 Hartree

Zero-point correction = 0.292367 (Hartree/Particle)

Ch4(radical)

C	5.072955	0.592649	-0.046673
C	5.317952	-0.773326	0.067381
C	4.246904	-1.679525	0.126677
C	2.947427	-1.204413	0.071638
C	2.645867	0.168082	-0.043594
C	3.751801	1.064418	-0.102882

H	5.871418	1.326469	-0.095447
H	4.452666	-2.744115	0.215369
H	2.139834	-1.931671	0.120386
C	1.282752	0.720153	-0.106368
C	0.135769	-0.095783	-0.050627
C	-1.163143	0.399057	-0.109722
C	-2.368916	-0.381887	-0.068321
C	-3.629080	0.263548	-0.141672
C	-2.382524	-1.798551	0.041451
C	-4.831886	-0.460468	-0.115352
C	-3.572275	-2.504133	0.080154
H	-1.442292	-2.341707	0.100897
C	-4.811533	-1.853767	0.003550
H	0.291465	-1.166378	0.040163
H	-1.284352	1.473921	-0.200617
O	1.176100	2.029849	-0.220503
O	3.538547	2.383531	-0.214281
H	2.447493	2.426807	-0.234871
O	-3.677823	1.631726	-0.295760
C	-4.000847	2.338851	0.902040
H	-4.994242	2.056092	1.264339
H	-3.250784	2.143117	1.677767
H	-3.992679	3.401146	0.649634
O	6.565044	-1.322965	0.128569
C	7.682151	-0.449365	0.077449
H	8.564842	-1.086107	0.142099
H	7.704865	0.111646	-0.864132
H	7.675711	0.252618	0.919445
H	-3.551725	-3.589562	0.169080
H	-5.728648	-2.432688	0.029548
O	-5.970493	0.283300	-0.218796
C	-7.211558	-0.394243	-0.106539
H	-7.299413	-0.906258	0.858939
H	-7.980151	0.375711	-0.180994
H	-7.345917	-1.120360	-0.917000

Radical

E = -1076.02898969 Hartree

Zero-point correction = 0.322175 (Hartree/Particle)

Neutral optimized at radical anion geometry

E = -1075.88564462 Hartree

Zero-point correction = 0.324024 (Hartree/Particle)

Ch5(radical)

C	5.166160	0.451297	-0.010395
C	5.323925	-0.929120	0.009541
C	4.199701	-1.773582	0.026786
C	2.934599	-1.212362	0.022744
C	2.719563	0.181737	0.001519
C	3.876730	1.037647	-0.014085
H	6.013717	1.129636	-0.023272
H	4.338684	-2.852231	0.043448
H	2.081054	-1.887396	0.037401
C	1.391773	0.783916	-0.004340
C	0.187619	0.072337	0.003435
C	-1.070510	0.671168	0.002613
C	-2.334156	-0.014765	0.000548
C	-3.553852	0.721151	0.008569
C	-2.465917	-1.422923	-0.011620
C	-4.798965	0.090990	0.004222
C	-3.694627	-2.064836	-0.015753
H	-1.567708	-2.036722	-0.019142
C	-4.869572	-1.307512	-0.008122
H	0.261494	-1.010712	0.008886
H	-1.108397	1.755170	0.002319
O	1.343218	2.132555	-0.018270
O	3.748469	2.345954	-0.031727
H	2.361838	2.429868	-0.024569
O	-3.424488	2.078020	0.020889
C	-4.597769	2.873800	0.028262
H	-5.203432	2.700343	-0.869205
H	-5.203375	2.684047	0.922476
H	-4.255709	3.909137	0.037773
H	-5.704192	0.682479	0.010726

O	6.535863	-1.560706	0.014756
C	7.704538	-0.756978	-0.004529
H	8.546582	-1.449848	0.000512
H	7.746551	-0.137908	-0.908396
H	7.757792	-0.111277	0.879930
H	-3.759441	-3.151126	-0.025832
O	-6.042952	-2.006811	-0.013262
C	-7.258522	-1.276285	-0.010045
H	-7.344666	-0.641455	-0.900085
H	-8.055936	-2.019845	-0.019427
H	-7.350039	-0.658330	0.891268

Radical

E = -1076.03566938 Hartree

Zero-point correction = 0.323405 (Hartree/Particle)

Neutral optimized at radical anion geometry

E = -1075.89308990 Hartree

Zero-point correction = 0.324933 (Hartree/Particle)

Ch6(radical)

C	-4.958015	-0.426370	-0.017587
C	-5.046467	0.959267	0.029310
C	-3.881833	1.748492	0.051421
C	-2.646313	1.127443	0.028271
C	-2.501628	-0.274830	-0.021725
C	-3.698311	-1.073120	-0.045552
H	-5.838317	-1.061622	-0.035124
H	-3.968764	2.832052	0.089771
H	-1.760776	1.759677	0.050947
C	-1.206271	-0.943456	-0.036664
C	0.031428	-0.290852	-0.025819
C	1.256873	-0.953521	-0.017381
C	2.552145	-0.333023	-0.006897
C	3.731364	-1.141982	0.023984
C	2.741931	1.063915	-0.025252
C	4.990494	-0.560773	0.031242

C	4.010736	1.641757	-0.017156
H	1.883324	1.731514	-0.048365
C	5.148200	0.835225	0.009653
H	0.012175	0.794298	-0.019339
H	1.240989	-2.037870	-0.014864
O	-1.226978	-2.288347	-0.052887
O	-3.631459	-2.385327	-0.091717
H	-2.266427	-2.534791	-0.073763
O	3.523793	-2.494255	0.045429
C	4.660787	-3.338169	0.079731
H	5.289579	-3.198102	-0.808038
H	5.261499	-3.162259	0.980475
H	4.277294	-4.359040	0.093991
H	5.886115	-1.173385	0.053618
O	4.039280	3.012806	-0.037235
H	6.151190	1.248479	0.015832
C	5.308292	3.643472	-0.031585
H	5.112552	4.716166	-0.050373
H	5.875033	3.393940	0.873720
H	5.896581	3.366442	-0.914872
O	-6.224084	1.649132	0.061495
C	-7.432556	0.905987	0.041271
H	-8.237950	1.640375	0.072384
H	-7.516429	0.310096	-0.874998
H	-7.507199	0.245194	0.912736

Radical

E = -1076.03528311 Hartree

Zero-point correction = 0.323024 (Hartree/Particle)

Neutral optimized at radical anion geometry

E = -1075.88698444 Hartree

Zero-point correction = 0.324404 (Hartree/Particle)
